RESEARCH PROPOSAL ON MODELLING & CHARACTERIZATION OF ATMOSPHERIC PRESSURE PLASMA JET BASED ON DIELECTRIC BARRIER DISCHARGE

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1. OBJECTIVE

The main objective of this research work would be to model and characterize different electrode configurations of dielectric barrier discharge based atmospheric plasma jets(DBD-APPJ) at different operating parameters. The operating parameters like kind of gas, gas flow rates, frequency of pulse and applied voltage would be varied and a comparative study of various DBD based atmospheric pressure plasma jets would be done. The electrical characterization of DBD-APPJ would be done with the help of V-I measurements. The spectral characterization would be done using optical emission spectroscopy in the wavelength range from infrared to ultraviolet range. The emission spectrums of the plasma tell us about the plasma chemistry like the density of various excited states of gas atoms & also about the various metastable states. Modeling of various DBD-APPJ's would be done with the COMSOL MULTIPHYSICS software which is based on finite element method. Plasma module will be used to simulate DBD based discharges and fluid dynamics module will be used for incorporating the flow of gas. The results of both modeling and experiments would be correlated.

2. PREVIOUS WORK DONE ON DBD-APPJ

Electric discharge in gases occurs when electric current flows through a gaseous medium. The plasma is formed due to ionisation of the gas. Plasma discharges having different characteristics can be produced in lab [1]. The various types of discharges like corona discharge, glow discharge, arc discharge are distinguished by their current-voltage characteristics like current density, breakdown voltage and luminescence [2-3]. Dielectric-barrier discharge is the discharge between two electrodes separated by an insulating dielectric barrier. Originally it was called silent (inaudible) discharge or partial discharge.

DBD- APPJ is usually generated by applying high-voltage pulses (5–15 kV, 10–100 kHz). A process gas (e.g. -nitrogen, helium, argon or air) flowing past this discharge section(between ground & powered electrode) is excited and converted to the plasma state[4,5]. This plasma then passes through the jet head to arrive on the surface of the material to be treated.The jet head is at ground potential. In addition, jet head determines the geometry of the emergent beam. Several distinct features have made the non-thermal APPJ very appealing in practical applications. First being thermal non-equilibrium in these plasmas, second, the use of atmospheric pressure increases the opportunity of generating chemically active species (radicals) due to three body processes, such as excited dimmers and trimmers. Third, the use of atmospheric pressure greatly reduces the operational cost without the need of using sealed chambers, vacuum pumps, which are very expensive in procurement and maintenance.

The following electrode configurations of DBD APPJ shown in Figure 1 have been studied for various purposes like surface treatment, bio-medical applications etc.

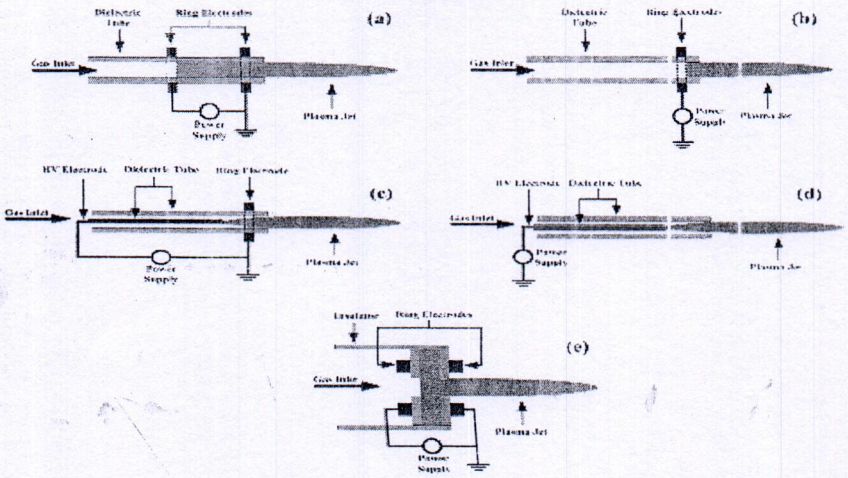

Figure.1 Various Electrode Configurations of DBD-APPJ

2.1 WORK DONE IN MODELLING

Liu and Neiger [6] proposed an electrical model of a DBD for arbitrary excitation voltage. Valdivia-Barrentos et al [7] have used the concept given by Liu and Neiger [6] to simulate the model by superimposing micro discharges on the displacement current waveform for different operating frequencies which does not consider the abrupt current increment produced by the change in the conductive process. Flores-Fuentes et. al [8] proposed a model using power law concept. Pal et. al [9] made an effort to understand a single peak discharge phenomenon based on an equivalent circuit model which has enabled them to characterize DBD's electrically and made it possible to obtain a large parameters instantaneously.

Initial work on static DBD discharge at pressures of the order of 10^3 Pa was done by Piquet [10] in COMSOL. The author has developed a Partial Differential Equation model of a plane excimer lamp (as shown in Figure.2) with working gas as Xenon. Different power supply modes are tested on this model and the densities of the gas discharge species as well as their efficiencies are computed as the ratio of the mean UV output power to the mean input electrical power. The model shown in Figure.2 was used to compute the efficiency of the excimer lamp for a sine waveform voltage source of 8 kV peak. The results of the experiments are presented in Figure.3 for frequencies between 50 kHz and 350 kHz.

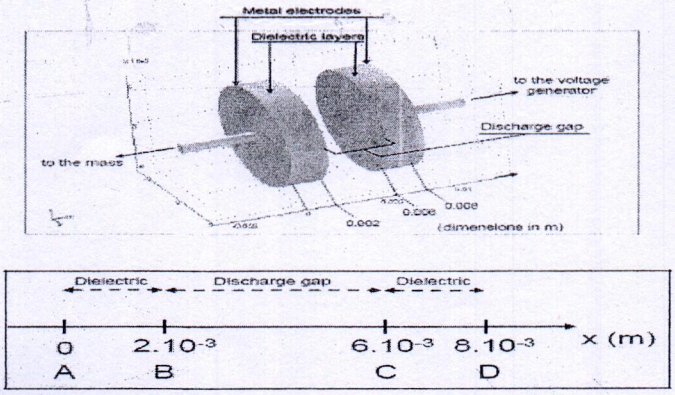

Figure.2 Discharge geometry

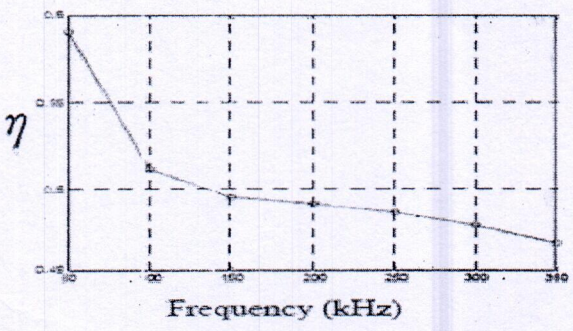

Figure.3 Efficiency Vs Frequency

In 2011 Kelly & Turner [11] developed the fluid model of the 2D cross section of an AC driven plasma at atmospheric pressure with geometry as shown in Figure 4. A 2D fluid model is solved for an Argon chemistry using COMSOL MULTIPHYSICS for a cross section of the inter-electrode region shown in Figure 5. Discharge of argon gas included species like electrons, Argon atomic ions and Argon metstables. Six reactions are included in this model with three electron impact reactions and two Heavy species reactions (Penning Ionization, Metastables quenching). The discharge is driven at 50 kHz frequency and with applied voltage of 0.75kV. The gap width is 2mm with dielectric material (ε_r= 10) on either side with thickness 1mm. The barrier length is 2cm. This work was done using argon gas but can be extended to other gases like nitrogen, helium and air.

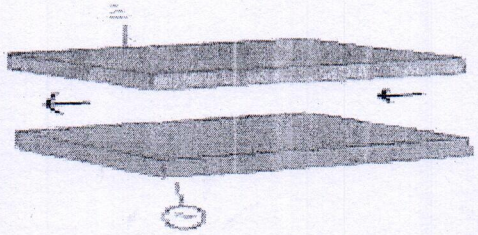

Figure.4 Plasma Jet source with driven and grounded electrodes and dielectric barrier.

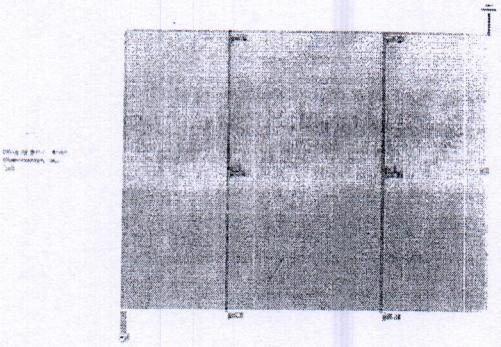

Figure.5 2D cross section of a Plasma Jet with driven and grounded electrodes

In 2006 C. Tendero et al.[12], had successfully modelled DBD reactor using COMSOL® code as shown in the figure 6.The reactor consists of a 120 mm long and 2 mm thick glass tube with a diameter of 30 mm. The stainless steel high voltage electrode is a 2 mm thick and 26 mm diameter disc. The space between high voltage electrode and the glass tube used as dielectric material is 2 mm. Under these experimental conditions, the discharge is filamentary. Pure air is injected in the gas inlet A while the air charged with the pollutant is introduced in the gas inlet B at 10 mm from the electrode. In the first step the hydrodynamics and the diffusion of the pollutant in the discharge region is simulated in 3D. In this domain very strong gradients of pressure and concentrations occur, however as this domain is axisymmetric a 2D model is used. Electrons react with air, forming the active species (O_3, O, singlet O, ions).Their species concentration is calculated by solving their equations of conservation in a kinetic model of 5 species and 6 reactions. The concentrations of the species obtained in this 2D model are used as inlet conditions in the next step, in the post discharge region where the active species formed in the discharge region react with the pollutant. As a result of these simulations the depletion of a pollutant in a DBD reactor was successfully simulated with a 3D model reactor using COMSOL® code.

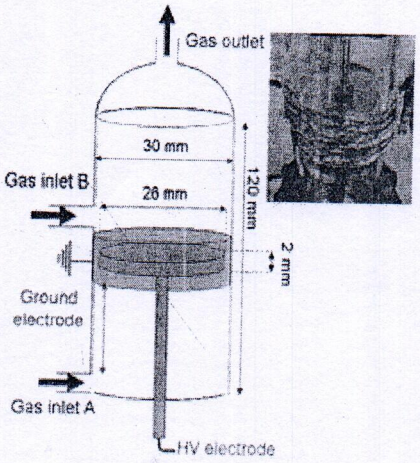

Figure.6 DBD reactor

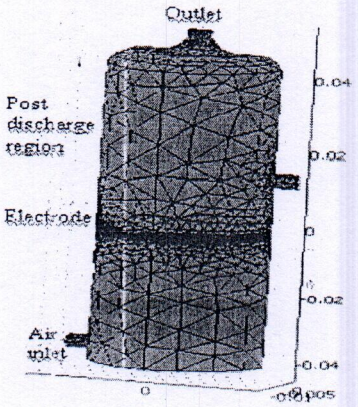

Figure.7 3D simulation domain and unstructured mesh

In 2006, Sakiyama and Graves [13] worked on modeling of RF (13.56 MHz) plasma needles based on a fluid model having He and a small fraction of N_2. They employed a two-dimensional fluid model with the LFA based on a finite element method using FEMLAB with MATLAB. They further investigated the two modes of the plasma needle operation. For low power (1 mW), the plasma needle operated in a corona-mode and above a certain threshold power (10 mW), a transition to a glow mode was observed. Their simulation results of the mode transition were confirmed by comparison with other groups' experimental studies [14]. DBD discharges in static mode has been simulated but DBD discharges including the flow of gas as jet has not been simulated in detail. It is proposed to simulate DBD-APPJ for different gases under experimental conditions.

2.2 WORK DONE ON CHARACTERIZATION OF DBD APPJ

Characterization of DBD-APPJ is very important to understand the intricate behavior of plasma jets. The DBD based jets are extremely dynamic & contains many active species hence it is imperative to understand the behavior of these jets with respect to various parameters like supply voltage, pulse frequency, pulse width, gas flow rate. Xiong et al[15] has done characterization of helium DBD APPJ with the electrode configuration given in figure 8.

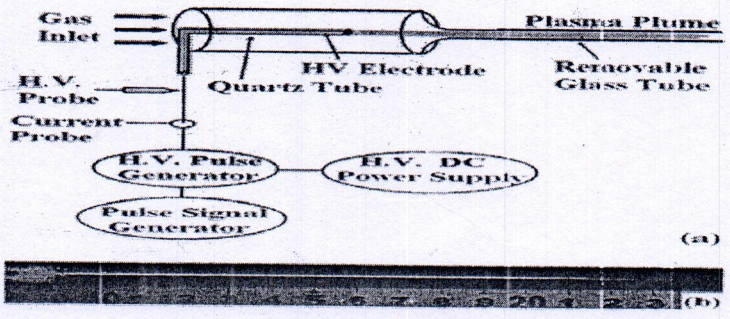

Figure.8 Va=9kV, P.W=4μs, Freq= 9KHz, He flow=0.5 l/min

In this experiment the authors have analyzed the length of the plasma jet with respect to the applied voltage, where it was observed that the length of plasma jet in open air increases with applied voltage till 8 kV and beyond that the plasma jet becomes less steep.

From the initial work done by Matveev & Silakov [16] it was observed that with the increase in applied voltage, both the positive primary and the negative secondary discharge currents are increased. It is imperative to note that the primary discharge current pulses I_{pri} appear at an early stage when the applied voltage is on the rise. Conversely, the secondary current pulses I_{sec} are always generated during the falling cycle of the voltage pulses.

Further temporal dynamics of the applied voltage and the discharge current for different values of applied voltage were studied by Motret et. al [17] using V-I characteristics. From the experimental results of Xiong et.al. [13] it was observed that the length of the plasma plume initially increases when the pulses become wider.But after pulse width of 4μs it was observed that further increase of pulse width had no effect on length of plasma jet. The effect of the pulse frequency repetition rate on the length of the plasma L_{pla} has also been studied by Woloszko et al [18]. It was found that there is a slight increase in the peak current value when frequency is increased. This was due to the primary discharge current appearing much earlier when the pulse frequency is higher.

2.3 APPLICATIONS OF PLASMA JET

Plasmas jets can be produced by various means, e.g. radio frequency, microwave frequencies, high voltage ac or dc, etc. During the non-equibilium processes both excited species and reactive gases may be produced (as well as ions and electrons) and it is these species that deserve particular attention for health care. Air plasma devices have been used in medical practice as a source of gaseous nitric oxide. The results of animal studies and clinical trials showed that NO-containing gas generated by plasma is effective in tissue disinfection and regulating inflammatory processes associated with acute and chronic wounds and respiratory problems.

Direct plasmas devices [19-21] use the skin (or other tissue) as an electrode so that the current produced passes through the body. Figure 9 shows the plasma produced by floating electrode dilelectric barrier discharge.

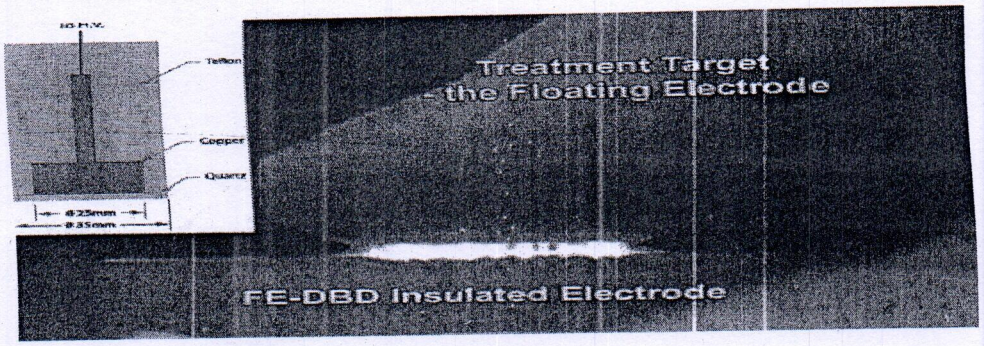

Figure.9 Plasma produced by the Floating-Electrode Dielectric Barrier Discharge (FE-DBD) electrode

Indirect plasmas are produced between two electrodes and are then transported to the area of application entrained in a gas flow. Different devices exist from very narrow 'plasma needles' to larger 'plasma torches' [22]. Figure 10 shows plasma needle set up where working gas is helium and RF source is used to generate the plasma.

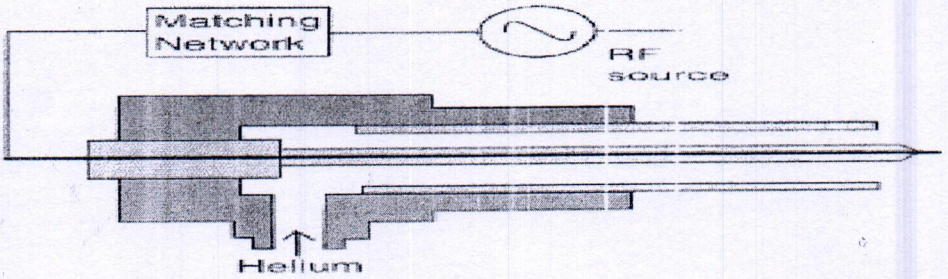

Figure.10 Plasma needle set-up

Plasma treatments are found to be the most effective in surface modifications such as creation of micro-roughness (ablation and etching) [22, 23]. Plasma treatment thus enhances adhesion, printability and dye uptake. Recent investigations also include the upgrading of wool and textiles and the plasma treatment of insulated wires and cables [24, 25]. Figure 11 shows the typical experimental set up of APPJ plasma set up where helium was initially used to generate the plasma using a RF power supply. This device was used for treating various textile fibers.

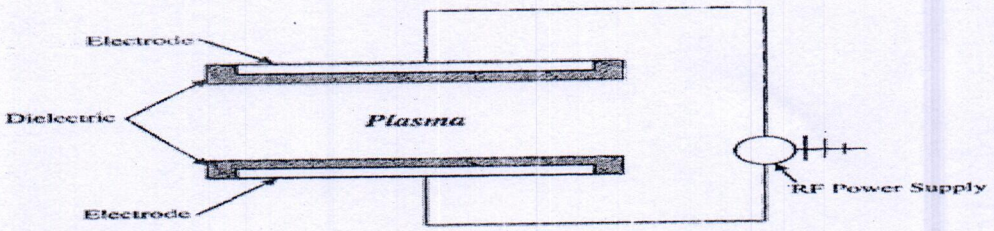

Figure.11 Atmospheric Pressure Plasma Treatment device

3. SCOPE OF WORK

It is proposed to simulate DBD- APPJ jets using two modules (Plasma module & fluid dynamics module) of COMSOL software and analyze the discharge of different gases e.g.

Argon, Nitrogen or Air under different flow rates. During the experiments various electrical parameters like applied voltage, pulse frequency, pulse width will be varied for different electrode configurations and the V-I characteristics will be measured. The spectroscopic study will be done to identify the different reactive species generated in these discharges.

4. APPROACH TO DO PROPOSED WORK

Experiments have already been carried out for the electrode configuration shown in figure 12 and cold plasma jet was generated at atmospheric pressure (Figure 13). As shown in the figure 12, the pin electrode acts as the powered electrode (sinusoidal pulse) and the ring electrode acts as ground electrode.

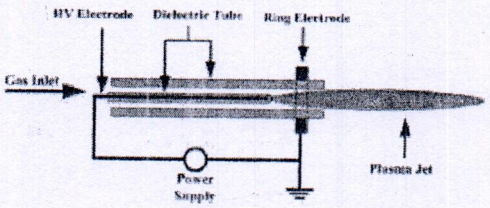

Figure.12 DBD-APPJ Electrode configuration

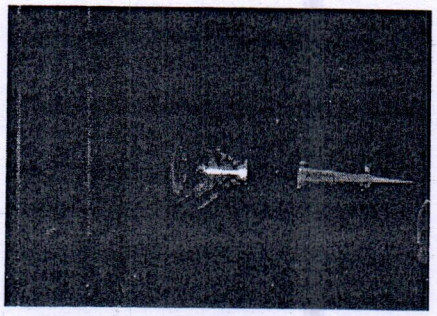

Figure.13 Generated Plasma Jet

4.1 MODELLING USING COMSOL MULTIPHYSICS

Since the APPJ is a highly dynamic and extremely chemically reactive it becomes necessary to model these discharges to understand them better. Comsol is a multi physics software that is based on Finite Element Method. It contains Plasma module in which we can perform 1D, 2D & 3D modeling and simulation of atmospheric pressure plasma jets using various electrode configuration at atmospheric pressure. The flow of the gas as in the case of APPJ can also be incorporated in the model by adding the fluid dynamics module to the simulation program. For each module there are a set of domain equations that are specified to characterize the physics behind the processes involved. The plasma module include all the necessary tools to model plasma discharges, beginning with a Boltzmann Equation, Two-Term Approximation solver computes the electron transport properties and source coefficients from a set of electron impact collision cross sections. The Boltzmann Equation, Two-Term Approximation interface makes it possible to determine many of the interesting characteristics of a discharge by providing input properties such as the electric field and the electron impact reactions that make up the plasma chemistry [26, 27].

4.1.1 Plasma Module Domain Equations

The electron density is calculated by

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot \Gamma_e = R_e - (\mathbf{u} \cdot \nabla) n_e$$

n_e denotes the electron density ($1/m^3$), R_e is the electron rate expression ($1/(m^3 \cdot s)$), Γ_e is the electron flux $1/(m^2 s)$. and **u** is the neutral fluid velocity vector (m/s). The subscript *e* refers to electron. The electron energy density is given by the following equation

$$\Gamma_\varepsilon = -(\mu_\varepsilon \cdot \mathbf{E}) n_\varepsilon - \mathbf{D}_\varepsilon \cdot \nabla n_\varepsilon$$

where, n_ε is the electron energy density (V/m^3), μ_ε is the electron energy mobility which is either a scalar or a tensor ($m^2/(V \cdot s)$). **E** is the electric field (V/m) and D_ε is the electron energy diffusivity (m^2/s). The subscript ε refers to electron energy [26, 27].The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \mu_e T_e, \mu_\varepsilon = \left(\frac{5}{3}\right)\mu_e, \mathbf{D}_\varepsilon = \mu_\varepsilon T_e$$

D_e is the electron diffusivity which is either a scalar or a tensor (m^2/s), μ_e is the electron mobility which is either a scalar or tensor ($m^2/(V \cdot s)$),T_e is the temperature of electron in electron volt [27].

4.1.2 Fluid Dynamics Module Domain Equations

It has equations, boundary conditions, and volume forces for modeling freely moving fluids using the Navier-Stokes equations, solving for the velocity field and the pressure.

The single-phase fluid-flow interfaces are based on the Navier-Stokes equations, which in their most general form are represented as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad (1)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} \qquad (2)$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T\right) = -(\nabla \cdot \mathbf{q}) + \tau : \mathbf{S} - \frac{T \partial \rho}{\rho \partial T}\bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla)p\right) + Q \qquad (3)$$

Where: ρ is the density, u is the velocity vector, *p* is pressure, τ is the viscous stress tensor, F is the volume force vector, C_p is the specific heat capacity at constant pressure, T is the absolute temperature, Q contains the heat sources, **q** is the heat flux vector, **S** is the strain-rate tensor. Equation (1) is the continuity equation and represents the conservation of mass.

Equation (2) is a vector equation and represents the conservation of momentum. Equation (3) describes the conservation of energy, formulated in terms of temperature.

4.2 INITIAL WORK DONE

Modeling using COMSOL was done for the electrode configuration as shown in Fig.12 for with & without flow of argon gas. Figure 14 shows the physical dimensions of DBD-APPJ configuration in mm.

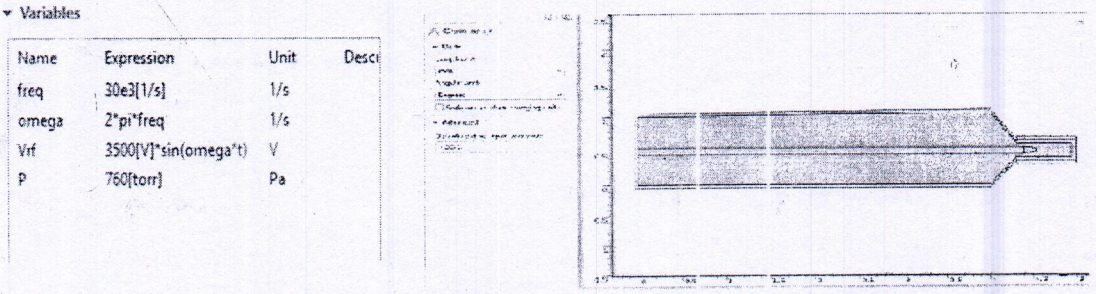

Figure.14 Modeling of DBD-APPJ without flow of argon gas

Figure 15 (zoomed portion of the above model) shows that electron density has reached order of 10^{18} per m^3 at $2.97x10^{-7}$ s.

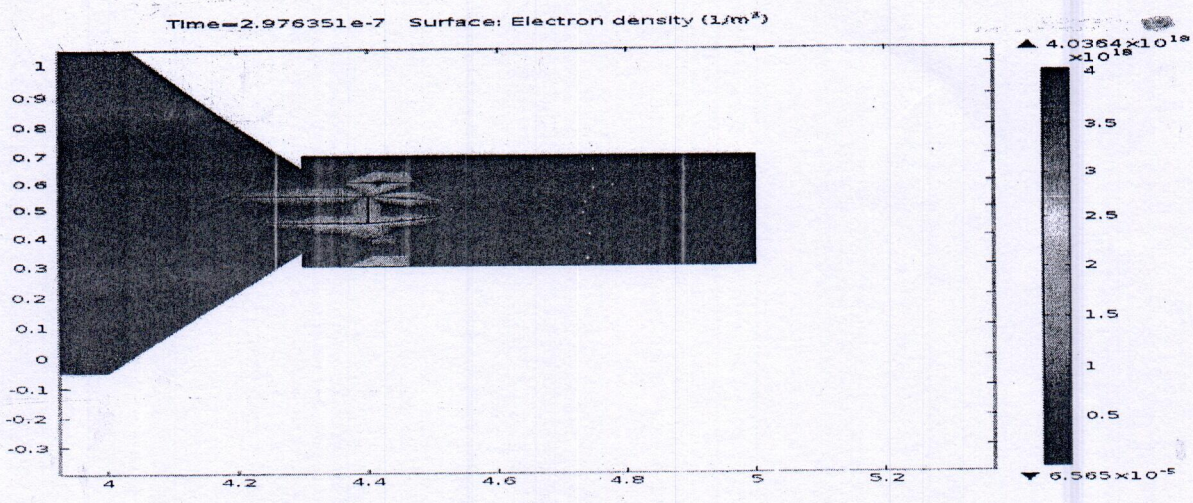

Figure.15 Electron density without flow of argon.

Figure 16 (zoomed portion of the above model) shows that electron potential has reached 196 V at 2.97×10^{-7} s.

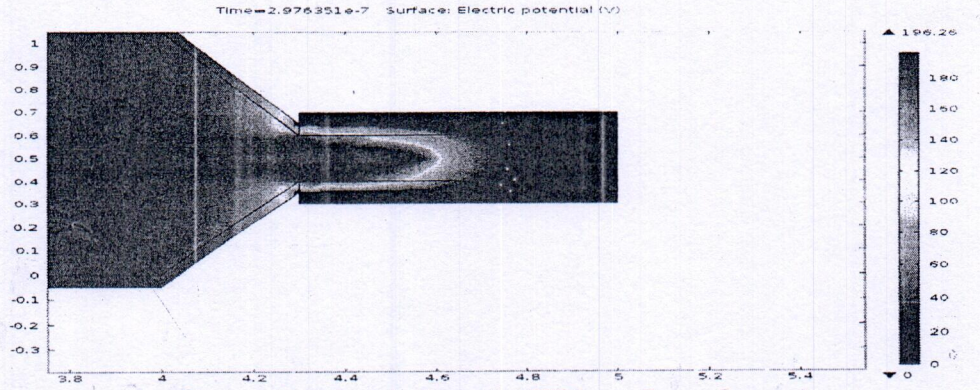

Figure.16 Electric Potential(Without flow of argon)

4.2.1 Modeling of (DBD-APPJ WITH FLOW of argon gas) using COMSOL

Figure 17 (zoomed portion of the discharge model shown in fig 14) depicts the electron density of the order of 10^{17} per m^3 at the time instant of 1.03 µs.

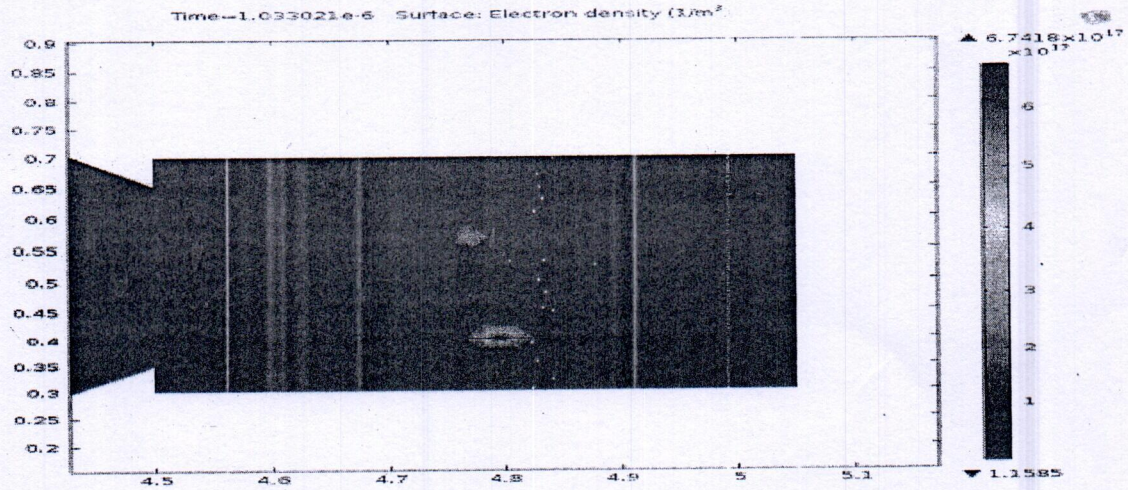

Figure.17 Electron density (with Ar flow)

Figure18 (zoomed portion of the discharge model Fig 14) shows the velocity of argon gas flow as 4.6 m/s at the instant of discharge.

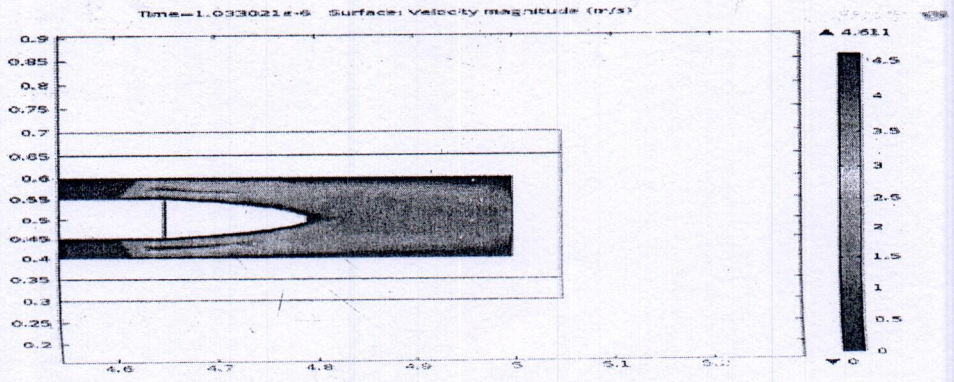

Figure 18. Velocity of argon flow

Figure.19 (zoomed portion of the discharge model Fig 14) gives the pressure value as $1.047*10^6$ Pa inside the discharge tube at the instant of discharge.

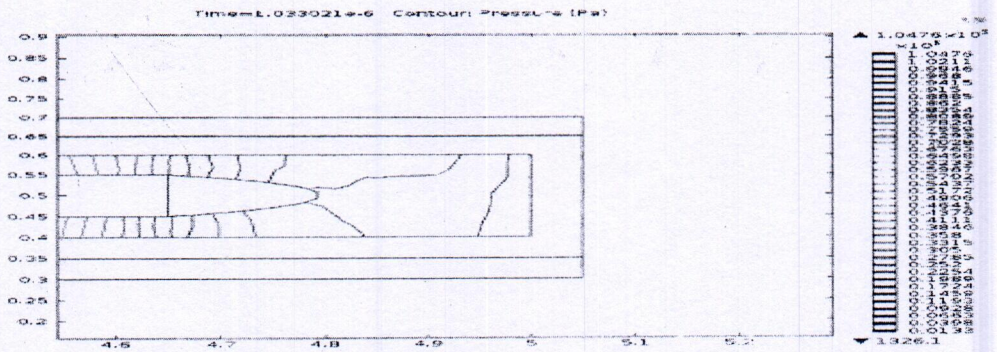

Figure19. Pressure inside discharge tube

4.2.2 V-I Characterization of DBD-APPJ

Figure 20 shows the experimental set up for measuring V- I characteristic of DBD-APPJ. The gas flow from the cylinders is controlled by manually operated valves but the gas into the DBD tube is controlled through a mass flow meter. One of the electrodes inside this DBD device is powered by a sinusoidal power supply .Voltage is measured with the help of high voltage probe. A high voltage single-ended probe is typically used for measuring ground referenced signals up to 40 kV. Rogowski coil is used to measure the discharge current. The experiments were carried out on argon based DBD-APPJ at CEERI-Pilani MWT lab are for the electrode configuration mentioned in Fig(14) using a pulsed power supply voltage of 5.5 kV, pulse width 3 μs and gas flow rate of 1 lit/min.

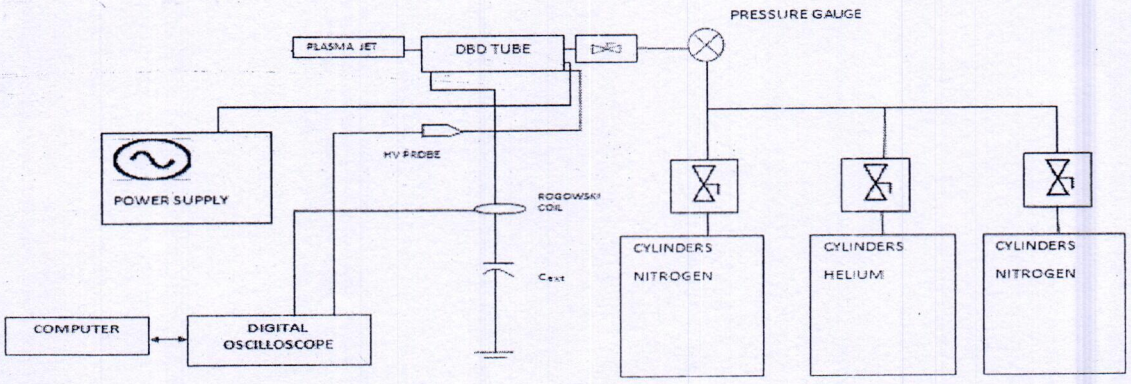

Figure.20 Experimental set up of study of V-I Characteristics

Figure 21 shows the V- I characteristic of discharge and measured current is 550 mA.

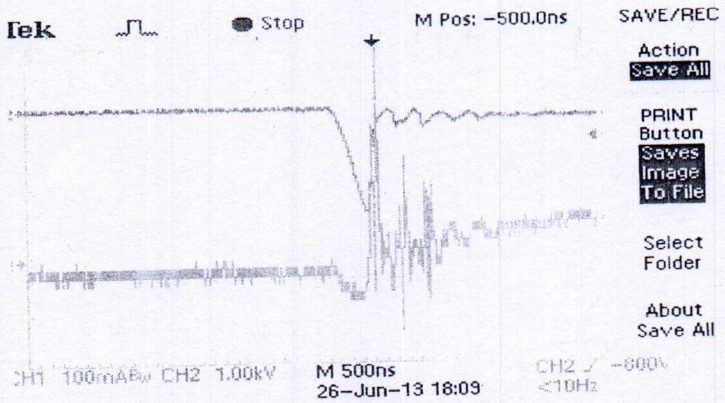

Figure.21 V-I characteristics of DBD-APPJ

4.2.3 Experimental Set-Up of Optical Emission Spectroscopy

Figure 22 shows the experimental set up of optical emission spectroscopy (OES). The photon intensity in the plasma jet is taken through an optical fiber to entrance slit of Czerny turner spectrometer which contains the photomultiplier tube that measures the intensity of photons corresponding to that wavelength. In the initial work, OES study was done for the electrode configuration shown in Figure 12.A typical spectrum recorded for DBD-APPJ experiment configuration is shown in figure 23.

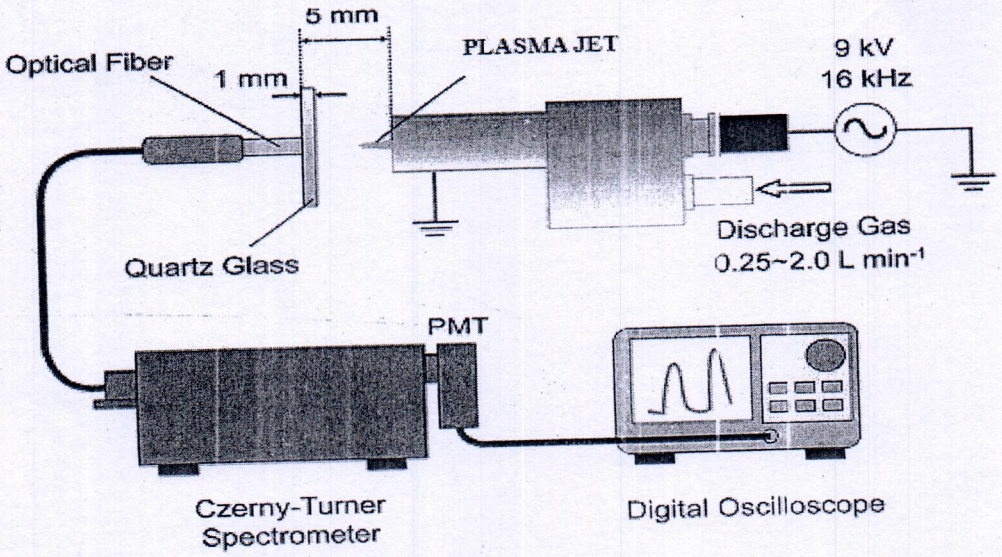

Figure.22 Experimental set up of OES of a DBD based Atmospheric Pressure Plasma Jet

A typical spectrum recorded for DBD- APPJ for argon gas. show that maximum intensity value is 2.55×10^6 at a wavelength of 308 nm.

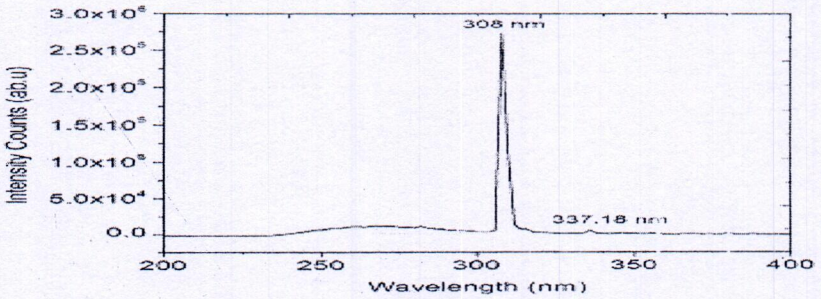

Figure.23 OES spectrum argon DBD-APPJ

5. WORK TO BE DONE

Modeling, V-I characteristics, and optical emission spectroscopy studies will be done for different electrode configurations of DBD-APPJ with different gases. Both the results of modeling and experiments would then be correlated for a better understanding of the behavior of DBD-APPJ's.

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